Ground state and low-lying excitations of the spin-1/2 XXZ model on the kagomé lattice at magnetization 1/3

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Abstract

We study the ground state and low-lying excitations of the $S = 1/2$ XXZ antiferromagnet on the kagomé lattice at magnetization one third of the saturation. An exponential number of non-magnetic states is found below a magnetic gap. The non-magnetic excitations also have a gap above the ground state, but it is much smaller than the magnetic gap. This ground state corresponds to an ordered pattern with resonances in one third of the hexagons. The spin-spin correlation function is short ranged, but there is long-range order of valence-bond crystal type.

Key words: Frustration, quantum paramagnet, valence-bond crystal

The spin $S = 1/2$ Heisenberg antiferromagnet on the kagomé lattice has been a focus of intense research during the past decade since it is a hot candidate for an exotic quantum ground state with a frustration-induced spin gap and a continuum of singlet excitations inside this gap (see [1, 2] for recent reviews). Furthermore, a clear plateau at one third of the saturation magnetization ($\langle M\rangle = 1/3$) is found for the $S = 1/2$ XXZ antiferromagnet in the presence of an external magnetic field on the kagomé lattice [3–6]. Here we discuss the nature of the ground state (GS) and low-lying excitations on this plateau.

Fig. 1 shows the spin-spin correlation functions determined numerically for the $S = 1/2$ Heisenberg model on an $N = 36$ kagomé lattice at $\langle M\rangle = 1/3$, *i.e.* in the GS of the $S^z = 6$ subspace. Note that the finite magnetization gives rise to a constant contribution $1/36 \approx 0.028$ in $\langle S_0^z S_j^z\rangle$ and $|\langle \vec{S}_0 \cdot \vec{S}_j\rangle|$. The nearest-neighbor correlations $\langle S_0^z S_1^z\rangle \approx -0.0506$ are consistent with an up-up-down spin arrangement around each triangle which would ideally give rise to a value of $-1/12 \approx -0.0833$. Around a hexagon, the sign of the correlations alternates antiferromagnetically from site to site. In particular at larger distances $\langle S_0^z S_j^z\rangle$ dominates over $\langle S_0^x S_j^x\rangle = \langle S_0^y S_j^y\rangle$. Despite the limited distances accessible on the $N = 36$ lattice, it is evident that the spin-spin correlations decay rapidly and are short-ranged.

Further insight can be gained by consideration of the XXZ model [6]. In the Ising limit, the GSs at $\langle M\rangle = 1/3$ are those states where around each triangle two spins point up and one down. These Ising configurations can be explicitly enumerated and the number of configurations $\mathcal{N}_{\rm conf}^{\rm I}$ determined for a given lattice size N (Table 1 lists a few values). The Ising configurations can be counted asymptotically exactly for large N (see [6, 7] and references therein), and one finds the growth law $\mathcal{N}_{\rm conf}^{\rm I} \sim (1.1137\ldots)^N$ on an N-site kagomé

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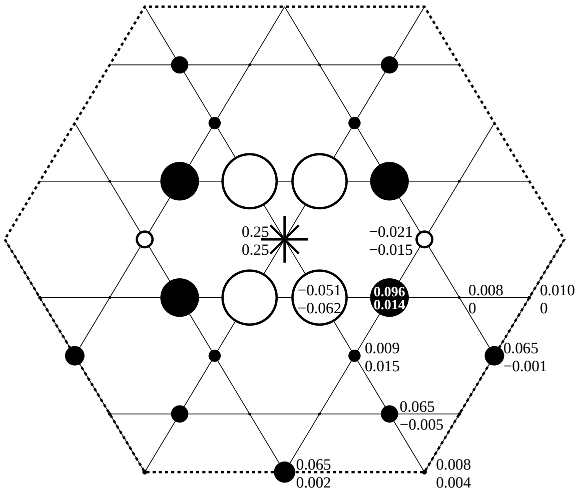
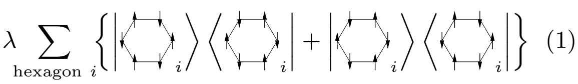


Fig. 1. $N = 36$ kagomé lattice. Dashed lines on opposite sides are identified by periodic boundary conditions. The radius of the circle at each site j shows the absolute value of the correlation function $|\langle \vec{S}_0 \cdot \vec{S}_j \rangle|$ for the $S = 1/2$ Heisenberg model at $\langle M \rangle = 1/3$; the big star denotes site 0. Numerical values for all inequivalent correlation functions are shown next to one selected site j. The upper number corresponds to $\langle S_0^z S_j^z \rangle$, the lower number to $\langle S_0^x S_j^x \rangle = \langle S_0^y S_j^y \rangle$.

lattice, in good agreement with the values in Table 1.

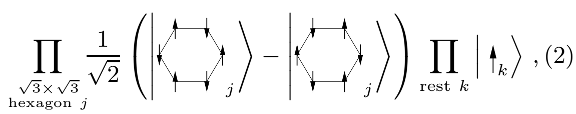
For $N \leq 36$, Table 1 also lists the number of non-magnetic states $\mathcal{N}^{\mathrm{H}}_{\mathrm{gap}}$ inside the magnetic gap of the *Heisenberg* model, defined by half the width of the $\langle M \rangle = 1/3$ plateau. These numbers are slightly smaller than $\mathcal{N}^{\mathrm{I}}_{\mathrm{conf}}$, indicating that $\mathcal{N}^{\mathrm{H}}_{\mathrm{gap}}$ and $\mathcal{N}^{\mathrm{I}}_{\mathrm{conf}}$ both grow exponentially with N in a very similar manner, and that the Ising configurations can be used to describe the low-lying states of the Heisenberg model.

Finite values of the XXZ anisotropy can be treated within perturbation theory around the Ising limit. The induced transitions between different Ising configurations are described by the effective Hamiltonian [6,8]



at lowest non-vanishing order and for $N \geq 36$. The sum in (1) runs over *all* hexagons i of the kagomé lattice. $\lambda > 0$ in the present context.

The effective Hamiltonian (1) is equivalent to a quantum dimer model on the hexagonal lattice whose GS is a valence-bond crystal (VBC) [8,9]. On the kagomé lattice, this VBC-type state can be visualized in terms of the following three-fold degenerate variational wave function



N	$\mathcal{N}^{\mathrm{H}}_{\mathrm{gap}}$	$\mathcal{N}^{\mathrm{I}}_{\mathrm{conf}}$	$E^{\mathrm{eff}}_{\mathrm{gs}}/\lambda$
18	13	20	
27	31	42	
36	100	120	$-4.690415760\ldots$
54		884	$-6.824621992\ldots$
81		15 162	$-9.970025439\ldots$
108		281 268	$-13.28992801\ldots$
144		13 219 200	$-17.63317376\ldots$

Table 1
Number of non-magnetic states $\mathcal{N}^{\mathrm{H}}_{\mathrm{gap}}$ in the magnetic gap of the Heisenberg model, number of GS configurations $\mathcal{N}^{\mathrm{I}}_{\mathrm{conf}}$ of the Ising model, and GS energy $E^{\mathrm{eff}}_{\mathrm{gs}}$ of (1) for some lattice sizes N.

where the first product now runs over an ordered $\sqrt{3} \times \sqrt{3}$ pattern of non-overlapping hexagons j (see inset of Fig. 1 of [6]). From (2) one obtains the variational energy $-\lambda N/9$. Although this is only in moderate agreement with the numerically exact GS energies $E^{\mathrm{eff}}_{\mathrm{gs}}$ of (1) shown in Table 1, the variational wave function (2) is still qualitatively correct [8,9].

The correlation functions shown in Fig. 1 for the *Heisenberg* model are very similar to those of the VBC GS of the effective Hamiltonian (1). Further evidence that the Heisenberg model and the vicinity of the Ising limit belong to the same phase is provided by the behavior of the overlap of the corresponding wave functions as a function of the XXZ anisotropy parameter and comparison of the spectra of the lowest excitations obtained numerically for the $N = 36$ kagomé lattice [6].

To summarize, the $S = 1/2$ Heisenberg antiferromagnet on the kagomé lattice has a three-fold degenerate GS of VBC-type at $\langle M \rangle = 1/3$ and a small gap to all excitations, although there are exponentially many non-magnetic states inside the magnetic gap.

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